Lipid Isomer Separation Using Travelling Wave Cyclic Ion Mobility Mass Spectrometry

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Introduction

- Galactosylceramide (GalCer) and glucosylceramide (GlcCer) are isomers and only differ in the position of the hydroxy group at the C-4 (Figure 1).
- Ganglioside GD1a and GD1b differ in the composition and sequence of sialic acid (Figure 1).
- A slight difference in chemical composition and molecular conformation contribute to profound differences in their physicochemical properties and biological functions.
- Here we Therefore, it is very important to separate these isomers to understand their biological role and function.
- Demonstrate the complete separation of these lipid isomers only possible with the multi-pass capability of the SELECT SERIES[™] Cyclic[™] ion mobility spectrometer (cIMS).



Figure 1. Chemical structure of the analyzed lipid isomers.

Experimental

- GalCer d18:1/18:0, GlcCer d18:1/18:0, ganglioside GD1a (d18:1/18:0) and GD1b (d18:1/18:0) were purchased from Avanti Polar Lipids and a final concentration of 1ng/µL was prepared. Samples were infused at 5µL/min into the ESI source of the cIMS.
- Different adduct ions were selected in the quadrupole and transferred to the cyclic mobility cell for multiple passes.

Results

GalCer and GlcCer Isomer Separation



Figure 2. Arrival Time Distribution for the separation of GalCer (d18:1/18:0) and GlcCer (d18:1/18:0) [M-H]⁻ m/z 726.5440 mixtures using 1(A), 5(B), 10(C), and 20(D) passes of the ion mobility device.



Figure 3. Arrival Time Distribution for the separation of individual GalCer (A), GlcCer (B) or the equimolar mixture of the two ceramides (C) using 20 passes of the ion mobility device.



Results

Ganglioside GD1a and GD1b Isomer Separation



Figure 4. Arrival time distribution for the separation of GD1a (d18:1/18:0) and GD1b (d18:1/18:0) at m/z 917.488 [M-2H]⁻² mixtures using (A) 1 pass, (B) 2 passes, (C) 3 passes, (D) 4 passes, and (E) 5 passes of the ion mobility device.



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Figure 5. Arrival time distribution for the separation of individual (A) GD1a (d18:1/18:0), (B) GD1b (d18:1/18:0), or (C) the equimolar mixture of the two ganglioside isomers at m/z 917.488 [M-2H]⁻² using five passes of the ion mobility device.

Conclusions

- The cIMS has a unique multi-pass cyclic ion mobility capability, to scale ion mobility resolution to meet a given challenge.
- The GalCer (d18:1/18:0) and GlcCer (d18:1/18:0) isomers were base line resolved using twenty passes of the IM cell, with IMS resolution of 290 $\Omega/\Delta\Omega$.
- The ganglioside isomers GD1a (d18:1/18:0) and GD1b (d18:1/18:0) were successfully resolved using 5 passes of the IM cell with IMS resolution of 145 Ω/ΔΩ.
- The scalable increased ion mobility resolution is useful to separate lipid isomers

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